

**NASA
Technical
Paper
2654**

December 1986

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Published for the NASA Administrator
by the NASA Technical Paper Series
Office of Technical Services
Washington, D.C. 20546
N7-14134

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Parametric Differentiation**

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Summary

Some path-following techniques are described and compared with other methods. Use of multipurpose techniques that can be used at more than one stage of the path-following computation results in a system that is relatively simple to understand, program, and use. Comparison of path-following methods with the method of parametric differentiation reveals definite advantages for the path-following methods. The fact that parametric differentiation has found a broader range of applications indicates that path-following methods have been underutilized.

Introduction

Considerable literature exists on path-following theory and methods (see, for example, ref. 1 and refs. included therein). An outstanding example is the paper by Keller (ref. 1, pp. 359–384) which includes, not a single metric in the domain space, but a general metric form, and no less than four techniques for locating bifurcating branches. Furthermore, the arc length normalization technique used by Keller eliminates the singularity at a turning point.

The path-following methods used in the present investigation are somewhat different from those described by Keller. The approach is simple in application, yet versatile, and requires a conservative amount of programming.

The great variety of problems to which some path-following techniques are applied preclude a categorical assertion that any one technique or system of techniques is optimal. A certain class of problems, for example, is concerned with bifurcation phenomena as such and the problems associated with obtaining convergent solutions in the vicinity of the singular point. For such problems, few path-following concepts are involved, and the methods described herein may not be helpful. These methods are directed toward problems, such as the majority of those discussed in the references, that involve path-following techniques: predictor and corrector methods; location and classification of singular points; methods for stepping through singular points; and locating secondary branches and disconnected solution sets.

The path-following literature appears to have focussed on the bifurcation theory and a restricted class of physical problems that have bifurcating solutions, such as beam buckling (Reiss, ref. 1, pp. 37–71), chemical reactors (Ray, ref. 1, pp. 285–315), Bénard convection (ref. 2, pp. 562–565), and Taylor-Couette flow (ref. 3, pp. 575–581). On the other hand, the closely related method of parametric differentiation (MPD) has been applied to a greater variety of problems. A partial listing of a 1985 li-

brary computer search revealed over 30 publications reporting on MPD analysis of problems involving radiation gas dynamics, ignition and combustion, solution of nonlinear Volterra integro-differential equations, nonlinear noise propagation, transonic airfoil and wing flows, unsteady transonic flows, internal transonic flow, compressible boundary layers, boundary layers with blowing, magnetofluid dynamics, and structural optimization.

However, there are inherent problems with MPD, both theoretical (it yields an approximate solution) and in its implementation. It will be shown that these problems are overcome by using path-following methods. Consequently, a large class of problems becomes subject to essentially exact solution.

Symbols

B	real Hilbert space
D	value of determinant obtained by discretizing L
F	function defining nonlinear source term in equation (16a)
f	function of x
h	$= \delta f$, variation of f
L	linear operator obtained by linearization of Q
MPD	method of parametric differentiation
P, G, z, q, H	functions used to define F (eqs. (16b) through (16g))
Q	differentiable nonlinear operator on $B \times R$
R, R^n	real one- and n -dimensional space
r	perturbation function
s	"arc length" on solution path in $B \times R$
x	independent variable
Δ	increment in parameter
δ	variation of function or operator
ϵ	coefficient (eq. (24))
θ	homotopy parameter
λ	real parameter
λ_a, λ_b	values of λ that bracket λ_c , $\lambda_a < \lambda_c < \lambda_b$
λ_c	estimated or actual critical (singular point) value of λ

ρ residual of nonlinear operator equation

$\| \cdot \|$ denotes the L_2 -norm in real Hilbert space

Subscripts:

i number of step along path

0 starting condition

1,2 conditions after first and second calculation steps, except in equations (29) through (31) where the subscripts denote different parameters

Primes with a symbol indicate differentiation with respect to independent variable x .

Analysis

Basic Path-Following Equations

It is assumed that the nonlinear operator $Q[f, \lambda]$ is defined on $B \times R$ where B is a real Hilbert space and R is the real line and that Q is continuously differentiable with respect to λ and has a Gateaux variation with respect to f . It is required to solve

$$Q[f, \lambda] = 0 \quad (1)$$

for a range of values of λ , given a starting solution $f_0(x)$ at λ_0 :

$$Q[f_0, \lambda_0] = 0 \quad (2)$$

(It will be shown later that it is sufficient to have only an approximate solution to begin the procedure.) If the parameter is incremented to $\lambda_1 = \lambda_0 + \Delta\lambda$ then, in general,

$$Q[f_0, \lambda_1] \approx Q[f_0, \lambda_0] + \frac{\partial Q}{\partial \lambda} \Delta\lambda \neq 0 \quad (3)$$

The first variation of the operator Q :

$$\delta Q = L[f_0, h; \lambda_0] \quad (4)$$

is a linear operator operating on the variation $h(x)$ of $f(x)$,

$$f_1 = f_0 + h \quad (5)$$

Then

$$Q[f_1, \lambda_0] \approx Q[f_0, \lambda_0] + L[f_0, h; \lambda_0] \quad (6)$$

If both f and λ are incremented simultaneously, then

$$Q[f_1, \lambda_1] \approx Q[f_0, \lambda_0] + L[f_0, h; \lambda_0] + \frac{\partial Q}{\partial \lambda} \Delta\lambda \quad (7)$$

Since the first term on the right vanishes, equation (1) is satisfied approximately for f_1, λ_1 provided that

$$L[f_0, h; \lambda_0] + \frac{\partial Q}{\partial \lambda} \Delta\lambda = 0 \quad (8)$$

Equation (8) is a linear equation for the variation h which, by equation (5), yields the approximate solution f_1 at $\lambda_1 = \lambda_0 + \Delta\lambda$. If this process is continued several times until λ is no longer close to λ_0 , then the cumulative error becomes unacceptable. Therefore, it is necessary to provide a means of eliminating the error at any step along the solution path. This elimination is accomplished by a corrector calculation as follows.

Calculate the residual of the *nonlinear* equation (1):

$$\rho(f_1, \lambda_1) = Q[f_1, \lambda_1] \quad (9)$$

Hold λ constant at $\lambda = \lambda_1$ and calculate the variation h that satisfies

$$L[f_1, h; \lambda_1] = -\rho \quad (10)$$

Then the function $f_{1c} = f_1 + h$ satisfies

$$Q[f_{1c}, \lambda_1] \approx Q[f_1, \lambda_1] + L[f_1, h; \lambda_1] = 0 \quad (11)$$

This procedure can be iterated to drive the residual to machine zero at $\lambda = \lambda_1$.

It is important to observe that neither equation (8) nor equation (10) need be formulated in terms of the inverse operator L^{-1} . They can be solved by any convenient numerical formulation, either explicit or implicit. Thus, near-singular problems, in which the highest derivative term is small, can be treated without the difficulties that arise in such methods as that of Adomian (ref. 3).

Singular points occur where the linear operator L vanishes:

$$L[f, h; \lambda] = 0 \quad (12)$$

A singular point may correspond to a bifurcation or a turning point of the solution path in the cross-product domain space. Considerable literature (ref. 4, for example) exists on the mathematics of bifurcation and solutions in the vicinity of a singular point. This theory is not repeated herein inasmuch as the primary concern of the present study is that of specific path-following computational techniques.

It is useful to define a kind of arc length to describe distances along the solution path in $B \times R$. Let $\| \cdot \|$ denote the L_2 -norm in B ,

$$\|f\| = \int f^2 dx \quad (13)$$

Then the arc length in the domain space $B \times R$ can be defined by

$$ds^2 = \|\delta f\|^2 + (d\lambda)^2 \quad (14)$$

If several parameters $\lambda_1, \lambda_2, \dots, \lambda_n$ are involved, the ordered array of parameters represents a vector λ in R^n . Then the domain space is $B \times R^n$ and the arc length is

$$ds^2 = \|\delta f\|^2 + |d\lambda|^2 \quad (15)$$

Equation (14) and its approximation obtained by replacing the differentials with finite increments are somewhat similar to the arc length normalization equations (2.10c) and (2.10d) of Keller (ref. 1, pp. 359-384). Setting $\theta = \frac{1}{2}$ in equation (2.10c) of Keller yields one half the value of ds^2 given by equation (14).

Path-Following Procedures

One of the primary goals of the present investigation was to establish a set of procedures that would be (1) relatively simple to understand, (2) simple to describe mathematically, and (3) require a frugal amount of computer code. Although it is recognized that some relatively recalcitrant problems may require more complex procedures, the methods described here have proved effective for the problems studied.

Model problem. To facilitate understanding of the methods to be described, the procedures will be illustrated by referring to a specific model problem. This example is of the same general type as that described by Keller (ref. 1, pp. 359-384), but with a different nonlinear term

$$\frac{d^2 f}{dx^2} + F(f, \lambda, x) = 0 \quad (16a)$$

$$F = 2q(\lambda) + \pi^2 H(\lambda) P\{G[z(f, \lambda, x)]\} \quad (16b)$$

$$P(G) = \sin G \quad (16c)$$

$$G(z) = z - z^2 \quad (16d)$$

$$z(f, \lambda, x) = f - q(\lambda) x(1 - x) \quad (16e)$$

$$q(\lambda) = \lambda^2 e^{-\lambda/2} \quad (16f)$$

$$H(\lambda) = \lambda \quad (16g)$$

$$f(0) = f(1) = 0 \quad (16h)$$

For this problem, the predictor equation (8) is

$$\frac{d^2 h}{dx^2} + \frac{\partial F}{\partial P} \frac{dP}{dG} \frac{dG}{dz} h + \left(\frac{\partial F}{\partial q} \frac{dq}{d\lambda} + \frac{\partial F}{\partial H} \frac{dH}{d\lambda} \right) \Delta \lambda = 0 \quad (17)$$

In equation (17), the first two terms represent the linear first variation of the operator of equation (16a)

$$L[f_0, h; \lambda_0] = \frac{\partial^2 h}{\partial x^2} + \frac{\partial F}{\partial P} \frac{dP}{dG} \frac{dG}{dz} (z(f_0, \lambda_0)) h \quad (18)$$

The residual, after the first predictor calculation, is obtained from the nonlinear equation (16a):

$$\rho(f_1, \lambda_1, x) = \frac{d^2 f_1}{dx^2} + F(f_1, \lambda_1, x) \quad (19)$$

Then, the linear corrector equation is obtained by combining equations (18) and (19)

$$L[f_1, h; \lambda_1] + \rho(f_1, \lambda_1, x) = 0 \quad (20)$$

which is the basic equation for the Newton procedure.

Path following in nonsingular regions. Special means are required to compute the solution paths in the vicinity of singular points, but for basic path following in nonsingular regions (see fig. 1), the predictor-corrector procedure described previously is effective. To complete one step along the path, the predictor equation (17) (fig. 2(a)) must be solved once and the corrector equation (20) perhaps several times.

Simpler versions of this procedure have also been used effectively. One of these is to "omit" the predictor step. Beginning with the initial solution f_0, λ_0 , one can increment λ and compute the residual $\rho(f_0, \lambda_1, x)$. Then, starting with arguments f_0, λ_1 , iterate the corrector equation

$$L[f, h; \lambda_1] + \rho(f, \lambda_1, x) = 0 \quad (21)$$

until the residual is reduced to the acceptable level. This procedure, which appears to omit the predictor step, is actually equivalent to using a "horizontal" predictor step (see fig. 2(b)). It has been used in the solution of systems of algebraic equations (ref. 5).

Another method, which provides a better predictor estimate than the horizontal predictor, but which still does not require the solution of a differential equation, is to use an extrapolation predictor. (See fig. 2(c).) After the first step has been completed, two solutions are available: f_0, λ_0 and f_1, λ_1 . The difference function $f_1 - f_0$ is obtained and the arc

length ds_1 is calculated by equation (14). Then λ is incremented to λ_2 , and the extrapolated predictor is

$$f_e = f_1 + \frac{\Delta_2 \lambda}{\Delta_1 \lambda} \delta f \quad (22)$$

where

$$\begin{aligned} \delta f &= f_1 - f_0 \\ \Delta_1 \lambda &= \lambda_1 - \lambda_0 \\ \Delta_2 \lambda &= \lambda_2 - \lambda_1 \end{aligned}$$

The initial solution for f_0, λ_0 is now no longer required in storage and can be written over. After the predicted solution has been corrected to obtain the solution f_2, λ_2 , the second arc length element ds_2 is calculated. Then the increment $\Delta_3 \lambda$ is chosen in such a way as to oppose any tendency for ds to increase or decrease, as for example

$$\Delta_3 \lambda = \Delta_2 \lambda \frac{ds_1}{ds_2} \quad (23)$$

This extrapolation procedure does not require additional programming, since the extrapolation routine is already needed as a means for "stepping across" singular points, as will be explained later.

Arc length control is incorporated automatically in the procedure of Keller (ref. 1, pp. 359–384), where the arc length normalization equation is included, along with the basic operator equation, as part of the nonlinear system to be solved.

There exist, of course, alternate methods of performing the corrector step besides the Newton procedure. Basic contraction mappings are discussed in reference 4 for solutions near a bifurcation point, and other procedures appropriate to specific problems are available. Where individual solutions of the corrector equation are costly in terms of computer time and storage, the corrector step is to be applied judiciously. For example, if an exact solution is required only at one specific value of λ , several predictor steps may be taken and then corrected without driving the residual to machine zero. That is, the corrector may be used simply to keep the solution path from wandering too far off course until the desired value of λ is obtained, and then the residual is driven to zero.

Locating and classifying singular points. Singular points, defined as points f, λ for which equation (12) holds, are determined in the numerical algorithm by the vanishing of the determinant of the matrix formed by discretizing L . For simple (first-order) or other odd-order bifurcations, the determinant changes sign as the singularity is crossed. This

convenient indicator is especially useful inasmuch as the vast majority of bifurcation problems of physical interest appear to involve simple bifurcation.

To predict the nature of a singular point, one can include a subroutine that is turned on by the operator determinant falling below a specified level in absolute value. The subroutine calculates the increments ΔD in the determinant values and computes and stores the ratios $\Delta D / \Delta \lambda$. If this ratio begins to increase in absolute value, no singularity exists. If it approaches zero linearly, a bifurcation is signaled. If it approaches zero quadratically, a turning point is signaled (ref. 2, pp. 490–491). Turning points are also signaled by the small values of $\Delta \lambda$ required to maintain uniform arc length increments. (See eq. (23).) It is important to observe that these indicators do not determine a singularity but only signal a potential singular point. For example, a turning-point signal would occur for a solution set satisfying equation (12) at an inflection point.

Computing bifurcating branches. Once a bifurcation point has been detected, a number of methods exist for locating the bifurcating branch. Keller (ref. 1, pp. 359–384) describes four methods. The first two of these methods were tried in the present investigation, but were eventually rejected (because of the complication of solving supplementary equations) in favor of the method of perturbing the operator to eliminate the singularity. This procedure is, in some respects, a simplified version of method II of Keller. This perturbation device is described in reference 2 (p. 491), and is applied by Reiss (ref. 1, pp. 37–71) to a buckling problem, for which the perturbation has a physical significance.

The method proceeds as follows (refer to fig. 3). Once a bifurcation point has been approximately located, say at λ_c , this critical value is bracketed by parameter values λ_a, λ_b , each several marching steps removed from λ_c , so that $\lambda_a < \lambda_c < \lambda_b$. Then the marching computation is returned to λ_a and a perturbation function is added to the operator equation. This function satisfies the boundary conditions (eq. (16h)) and vanishes at λ_a and λ_b . An example is

$$r(\epsilon, \lambda, x) = \epsilon (\lambda - \lambda_a) (\lambda_b - \lambda) x^2 (1 - x) \quad (24)$$

Notice that the function of x chosen for the perturbation function is different from that which occurs in the original equation (16e). The marching is recommenced at λ_a with a smaller step increment and with the perturbation function added to equation (1). If

the new path enters the domain of attraction of a supercritical bifurcating solution, then at λ_b where the perturbation vanishes, the solution will be on the secondary branch (fig. 3). If a supercritical bifurcating branch is not found, then the same procedure is employed to seek a subcritical branch by starting at λ_b and marching backward.

This perturbation technique possesses a theoretical weakness. In the subspace orthogonal to the primary path at the bifurcation point, there are an infinite number of directions. The actual bifurcation direction may not be near the direction represented by the solution of the perturbed equation. When the perturbation function in equation (24) is prescribed to be in the bifurcating direction, this perturbation procedure is similar to Keller's method II (ref. 1, pp. 359-384).

The bifurcation direction can be obtained with some effort. For simple bifurcation, it is the direction of the eigenfunction corresponding to the zero eigenvalue that causes L to vanish (see eq. (12)). For example, if the operator equation (eq. (1)) is

$$f'' + \lambda \sin f = 0$$

equation (12) becomes

$$h'' + \lambda(\cos f)h = 0$$

But the bifurcation occurs from the trivial solution $f = 0$; consequently, this equation is simply

$$h'' + \lambda h = 0$$

whose first nontrivial solution is at $\lambda = \pi^2$,

$$h = \sin \pi x$$

Consequently, an appropriate perturbation function for this problem is

$$r(\epsilon, \pi, x) = \epsilon(\pi - \lambda_a)(\lambda_b - \pi) \sin \pi x$$

Of course, very few problems of practical interest can be treated analytically in this manner. However, if a problem has been discretized so that equation (12) appears as a matrix equation, the zero eigenvalue that causes the singularity can be determined, and the bifurcation direction is that of the corresponding eigenvector.

This additional work is not actually required except perhaps for some extremely recalcitrant problem. It is not at all necessary for the perturbation function to correspond to the bifurcating direction but only to have some component in that direction.

The direction is corrected by the corrector step; consequently, considerable flexibility is permissible in selecting the perturbation function.

Another practical problem is that of selecting the sign and magnitude of the perturbation amplitude parameter ϵ . It may be necessary to perform a trial calculation to determine an appropriate magnitude for ϵ . Then, if the secondary branch is not found, a third calculation is carried out with the sign of ϵ switched.

Once a secondary branch has been located in this manner, one can determine if it crosses the primary branch or only intercepts it. If it crosses the primary branch, the solution can be continued across the primary branch by stepping across it. This is accomplished by prescribing a larger than usual extrapolation predictor when the solution approaches the estimated bifurcation point. Extrapolating well beyond the crossing point permits the corrector to correct to the new leg of the secondary branch (fig. 3).

Now the bifurcation location λ_c can be obtained with good accuracy by interpolating simultaneously along the primary and secondary branches in the $\|f\|, \lambda$ plot (fig. 3). An important consideration is that the precise location of the bifurcation point is not required to locate the bifurcating branch when the perturbation method is used. Other methods (Keller, ref. 1, pp. 359-384) require the bifurcation point location because the computation of the bifurcating branch must begin at this point. Precise location of the bifurcation point by a method such as interval-halving involves costly calculation in the near vicinity of the singular point where the convergence is often quite slow.

Continuation past turning points. Two methods have been utilized in the present investigation to continue a solution path through a turning point. The first is to extrapolate the solution obtained near the estimated turning-point location. Now a quadratic (e.g., parabola) extrapolation is required rather than the linear extrapolation that is used for stepping through bifurcation points. (See fig. 4.) This procedure has been used with some success in the present investigation. For some problems, however, the extrapolations were quite large, and the predicted solutions were so far from the actual path that the corrected solution would not converge to the new leg of the solution path. Naturally, such an extrapolation will fail to yield the path continuation if the singular point is an inflection point.

An alternate procedure—one that incorporates the perturbation technique used to locate bifurcating branches—has also been used successfully. Referring to figure 5, when the turning point is signaled, the

marching procedure is discontinued on the secondary branch and returned to the primary branch, well beyond the estimated singularity location. Now, the marching is initiated on the primary branch toward the estimated singular value of λ . Then, the equation is perturbed toward the unknown leg of the secondary branch. For the model problem (eq. (16)), this was accomplished by using the same perturbation function that was used to find the bifurcating branch but with ϵ having a larger value and the opposite sign. The perturbed solution jumps to the new branch (fig. 5). The perturbation is then eliminated, and the solution is continued both backward and forward along the new branch.

This perturbation technique worked with a relatively small perturbation amplitude, apparently because a secondary branch is a stronger attractor away from a turning point than near it. The technique is convenient to use since it already exists in the code as a means for locating a bifurcating branch. Furthermore, the perturbation method apparently is the only one available for locating disconnected solution sets (ref. 2, pp. 494–499). An interesting example of the occurrence of such disconnected solution sets in a physical context is reported in reference 4.

The method of Keller (ref. 1, pp. 359–384)—eliminating the turning-point singularity by augmenting the operator with the arc length normalization equation—was not used for several reasons. (1) It complicates the theory. (2) The singularities that occur for the augmented system are not necessarily the same as those for the original operator (ref. 1); one must monitor both systems for singularities. (3) In some problems, attempting to compute beyond the limiting λ value leads to computational difficulties. For example, reference 6 reports difficulties in applying the method when the predictor step exceeds the limiting value of λ .

Comparison of Path Following With Method of Parametric Differentiation

Path-following methods are related to several other procedures that attempt to solve nonlinear problems through a sequence of linear solutions. Such procedures include invariant embedding (ref. 7), quasi-linearization (ref. 8), the method of Adomian (ref. 3), and the method of parametric differentiation (MPD). Of these methods, MPD appears to have been used extensively. A pre-1985 library search generated a listing of nearly three dozen reports on applications of MPD.

Path-following studies appear to be limited primarily to mathematical investigations of bifurcation and turning-point phenomena and to a restricted

class of physical problems that display bifurcation and/or turning-point behavior. The latter includes thermochemistry in continuously stirred chemical reactors (ref. 1, pp. 285–315) and certain fluid dynamics problems of fundamental academic interest, such as Bénard convection and Taylor-Couette flow.

The MPD, on the other hand, has been applied to a large variety of problems. Some of these problems involve singular points (e.g., ref. 9), whereas others use MPD to arrive at solutions that are not sufficiently near the starting solution for the Newton-Raphson procedure to converge. In some investigations, the parameter occurs as a physical quantity (airfoil thickness or angle of attack, Damkohler number, etc.), whereas in others, it is introduced artificially. A clever use of the latter technique is described in reference 10.

However, the MPD possesses several inherent weaknesses, the most notable of which are that it does not guarantee an accurate solution and it does not provide a means of dealing with singular points. One can see how these difficulties arise, and how they can be overcome by path-following methods, by examining the MPD equations. Let the nonlinear operator Q depend directly and compositely on the parameter λ so that

$$Q[f(\lambda), \lambda] = 0 \quad (25)$$

A starting solution f_0, λ_0 is given. Differentiating equation (25) with respect to λ yields

$$L \left[f_0, \frac{df}{d\lambda}; \lambda \right] = 0 \quad (26)$$

where L is a linear operator operating on the function $df/d\lambda$. The solution path is continued starting from f_0, λ_0 by the relation

$$f_i = f_{i-1} + \frac{df}{d\lambda} \Big|_{i-1} \Delta\lambda \quad (27)$$

The similarity of equation (26) to the path-following equation (8) is obvious. Both are linear but the solution of equation (8) is the variation $h = \delta f$, whereas the solution of equation (26) is the derivative $df/d\lambda$. It is seen immediately that equation (27) fails at singular points where $df/d\lambda$ is not defined. Furthermore, the error that occurs in each step is cumulative, and consequently the degree of solution accuracy is uncertain after the solution has been continued for some distance. A number of attempts have

been made to minimize this problem. One method is to improve the estimate by including higher order terms in the series

$$f_i = f_{i-1} + \frac{df}{d\lambda} \Delta\lambda + \frac{1}{2} \frac{d^2f}{d\lambda^2} (\Delta\lambda)^2 + \dots \quad (28)$$

For each additional term in this series, another variation of the operator must be taken and an additional (linear) differential equation must be solved (one for $df/d\lambda$, one for $d^2f/d\lambda^2$, etc.).

Another method for reducing the cumulative error is to "correct" the initial slope $df/d\lambda$ at any point after the slope at the next point has been calculated by some kind of averaging. Various versions and combinations of these methods have been used. Reference 11 describes four such methods, but none guarantees that the computed path will not wander away from the true solution path. Reference 11 also indicates that accuracy is lost if the parameter step length is not correlated with the numerical scheme step size. Reference 11 also reports some problems with stability of solutions.

The path-following method attacks the problem of singular points by providing flags that signal their proximity and their nature, and by providing special tools for continuing the solution in the neighborhood of singular points. It solves the problem of solution accuracy by providing a corrector step for reducing the residual for the full nonlinear problem at any step along the solution path.

Another advantage of the path-following method concerns problems that involve more than one parameter. (See, for example, refs. 9 and 12.) If the parameters are varied simultaneously the MPD yields

$$L \left[f_j, \frac{\partial f}{\partial \lambda_j}; \lambda_j \right] + \frac{\partial Q}{\partial \lambda_j} = 0 \quad (j = 1, 2, \dots, n) \quad (29)$$

which is a set of n linear equations to be solved for $\partial f / \partial \lambda_j$. The continuation equation is

$$f_i = f_{i-1} + \sum_1^n \frac{\partial f_i}{\partial \lambda_j} \Delta \lambda_j \quad (30)$$

The path-following method yields, for the same problem,

$$L [f, h; \lambda_1, \lambda_2, \dots, \lambda_n] + \sum_1^n \frac{\partial Q}{\partial \lambda_j} \Delta \lambda_j = 0 \quad (31)$$

which is a single equation to be solved for the variation h .

One further advantage of the path-following method over the MPD concerns the starting solution f_0, λ_0 . For the MPD an accurate starting solution is crucial. However, with the path-following method one can start with an approximate solution at λ_0 and apply the corrector step until an accurate solution is obtained at λ_0 .

It is clear, therefore, that the path-following method has distinct advantages over the MPD, which has found many applications and has been applied innovatively in a broad range of physical and mathematical problems. It appears then that the path-following method has been underutilized as a theoretical and computational tool.

Concluding Remarks

Some path-following techniques have been described and compared with other methods. Emphasis in this investigation has been on multiuse techniques that can be used at more than one stage of the path-following computation. The use of an extrapolation predictor, for example, both eliminates the requirement for solving an operator equation for the predictor solution and provides a means for stepping across singular points. Use of the perturbation techniques for locating bifurcating branches reduces the requirement for obtaining the slowly converging solutions near bifurcation points. It is also useful for turning-point calculations and for locating disconnected solutions. This incorporation of multipurpose techniques results in a concise computer code that is relatively simple to use.

A comparison of the method of parametric differentiation (MPD) with the path-following method indicates distinct advantages for the path-following method both in efficiency and in accuracy. The method of parametric differentiation has been applied to a broad range of physics problems, whereas preoccupation with singular-point phenomena appears to have unnecessarily restricted the path-following methods to the relatively narrow class of problems that involves singular points.

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November 3, 1986

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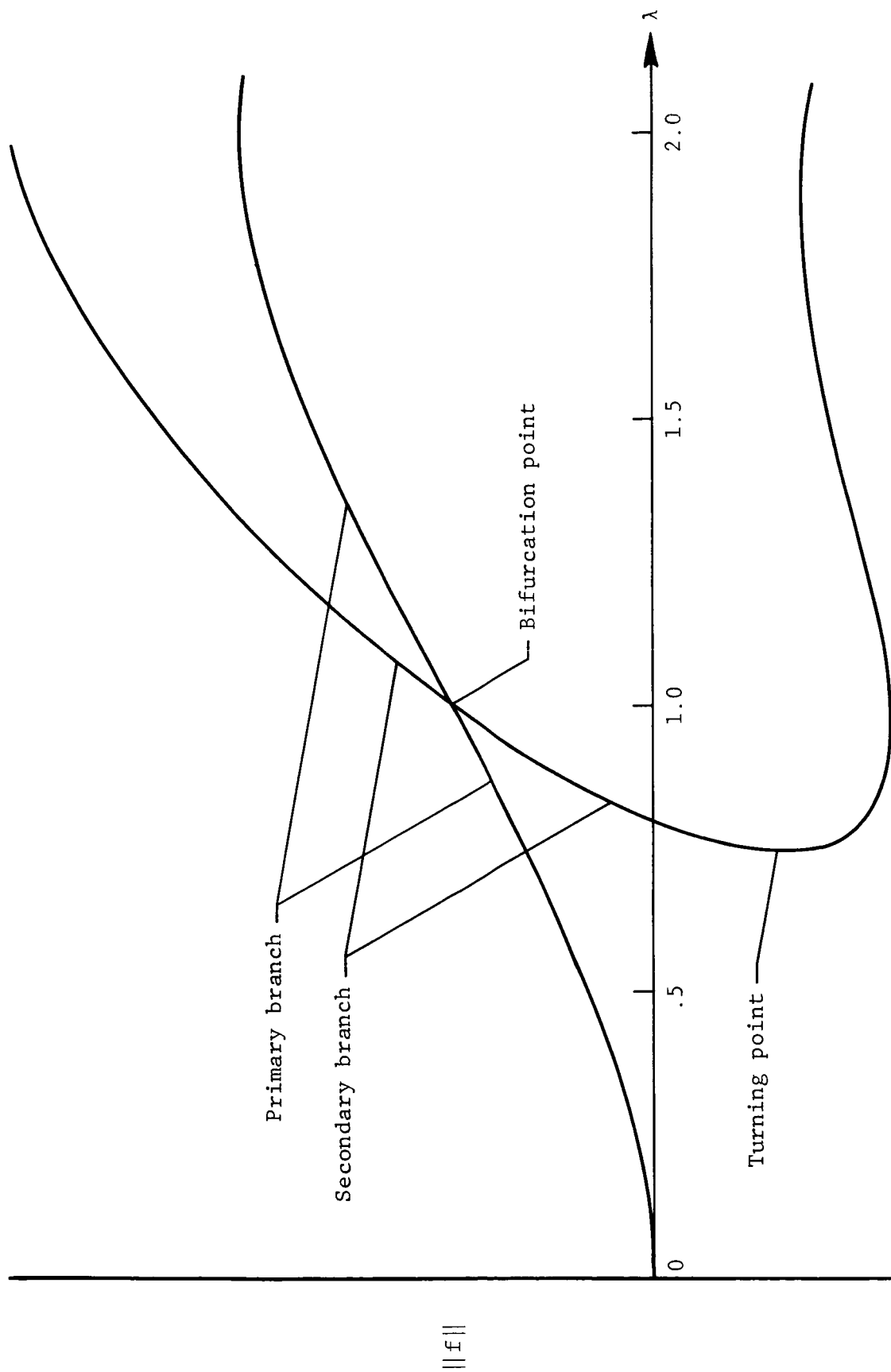
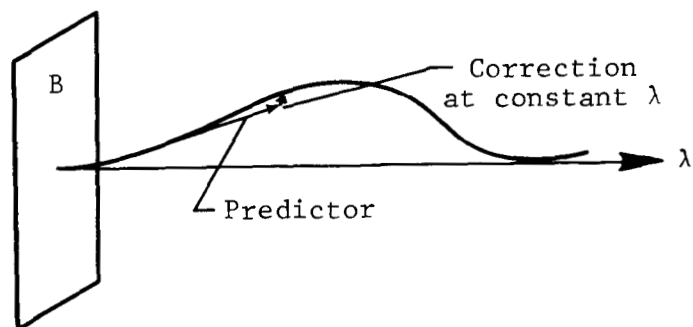
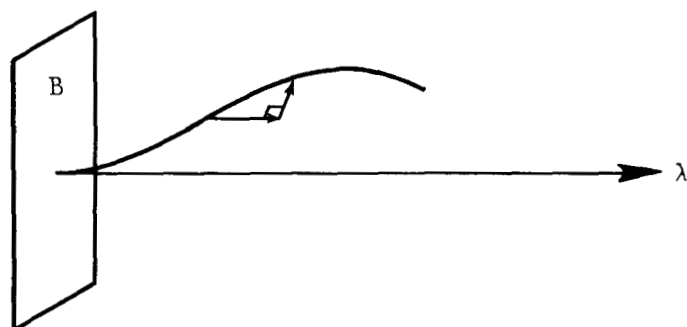


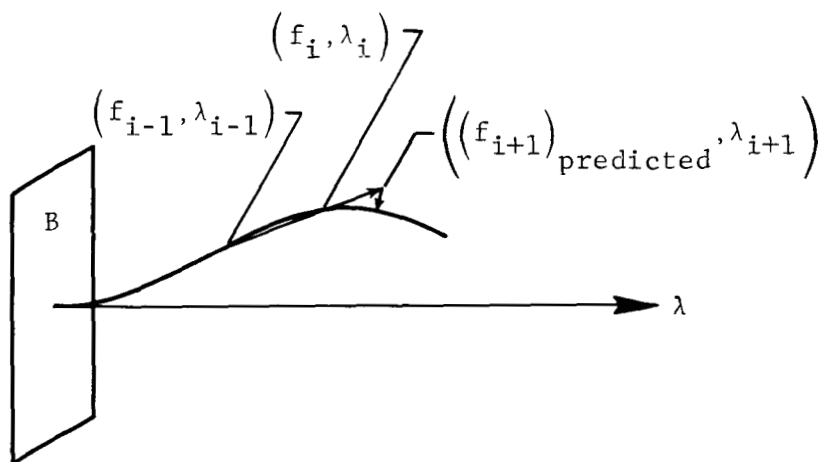
Figure 1. Structure of solution set for problem defined by equations (16a) to (16g), as indicated by plot of $\|f\|$ versus λ .



(a) "Tangent" predictor as solution of equation (8).



(b) Horizontal predictor: increment λ at fixed f .



(c) Extrapolation predictor.

Figure 2. Three types of predictor methods.

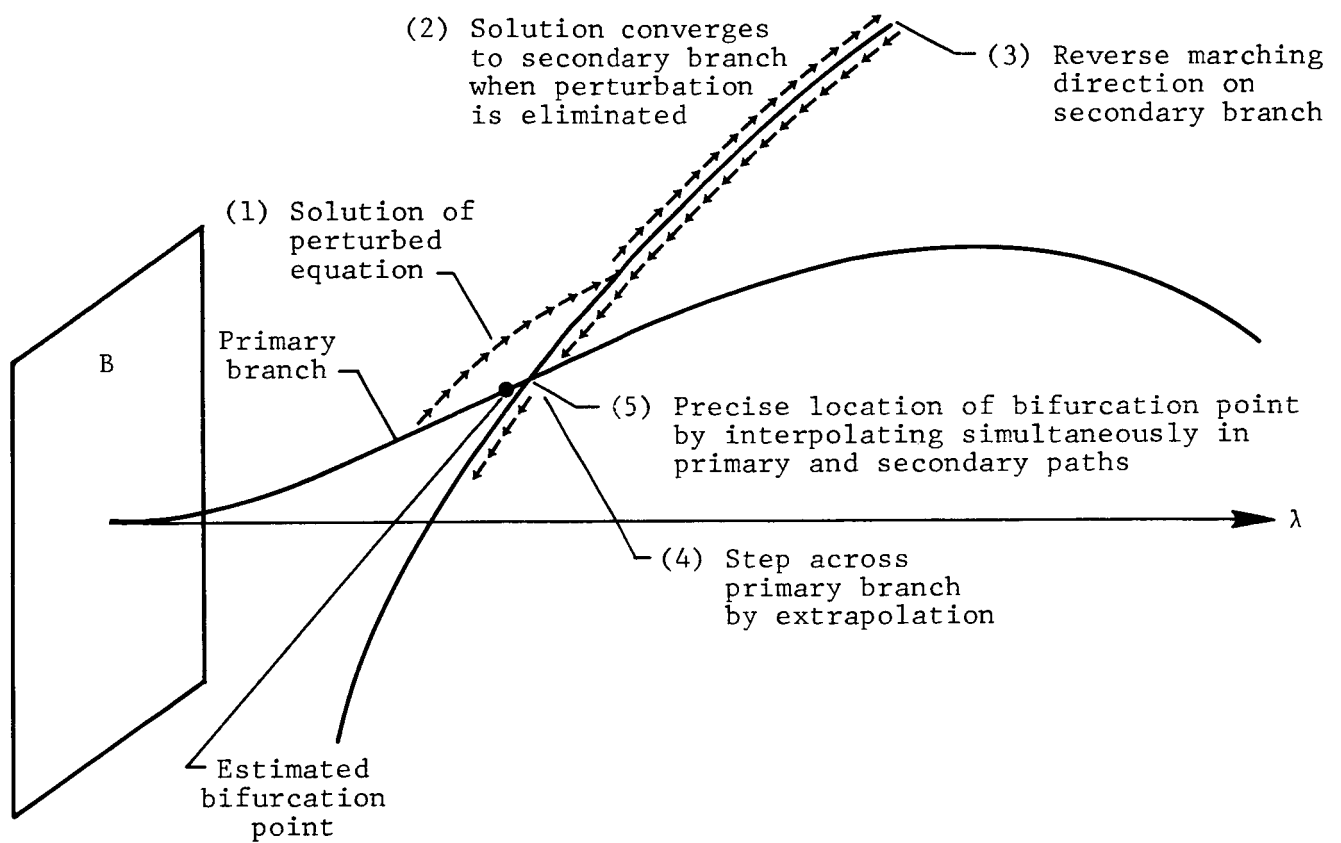


Figure 3. Perturbation approach to locating bifurcating branch and bifurcation point (after computing primary branch).

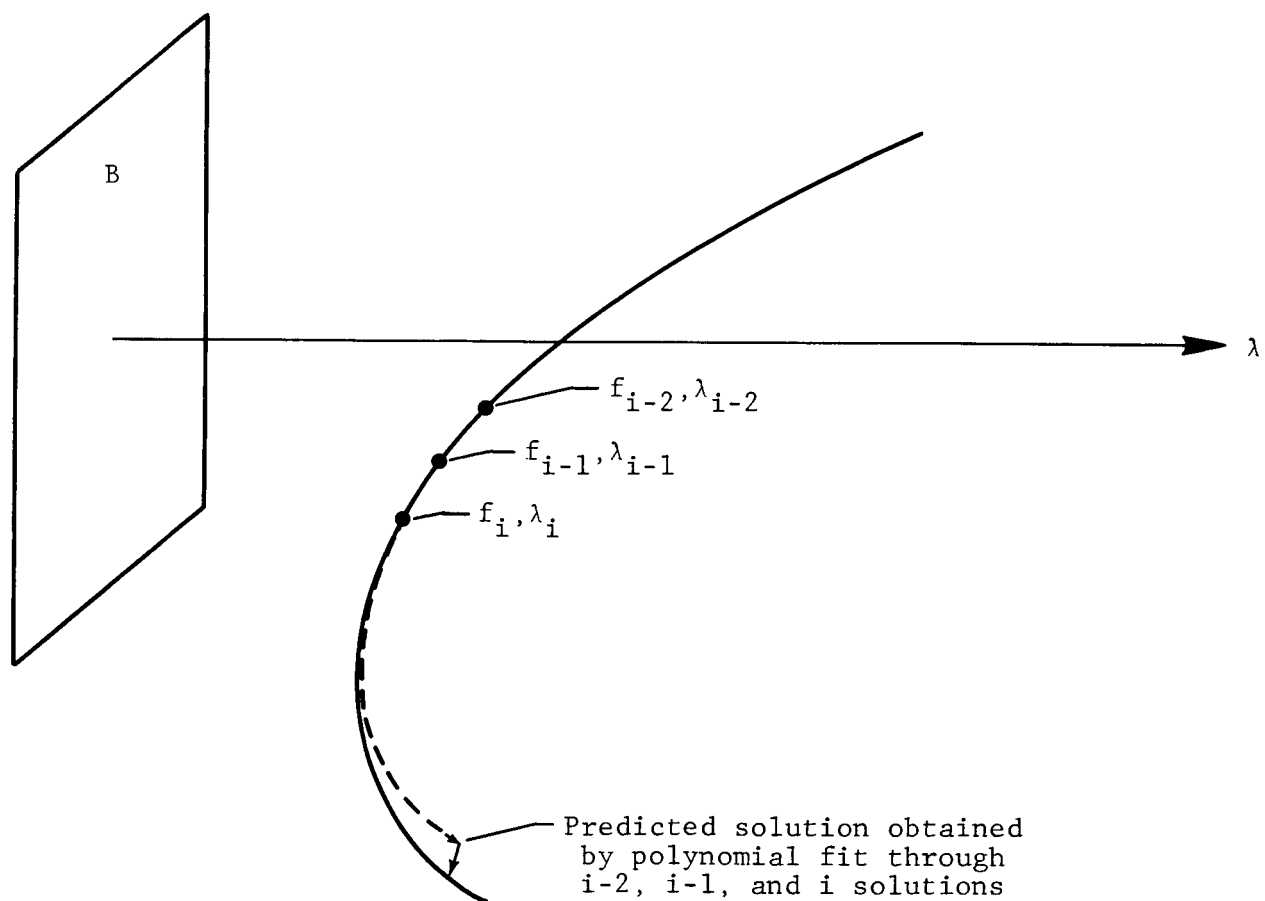


Figure 4. Method of obtaining predicted solution by polynomial extrapolation through turning point.

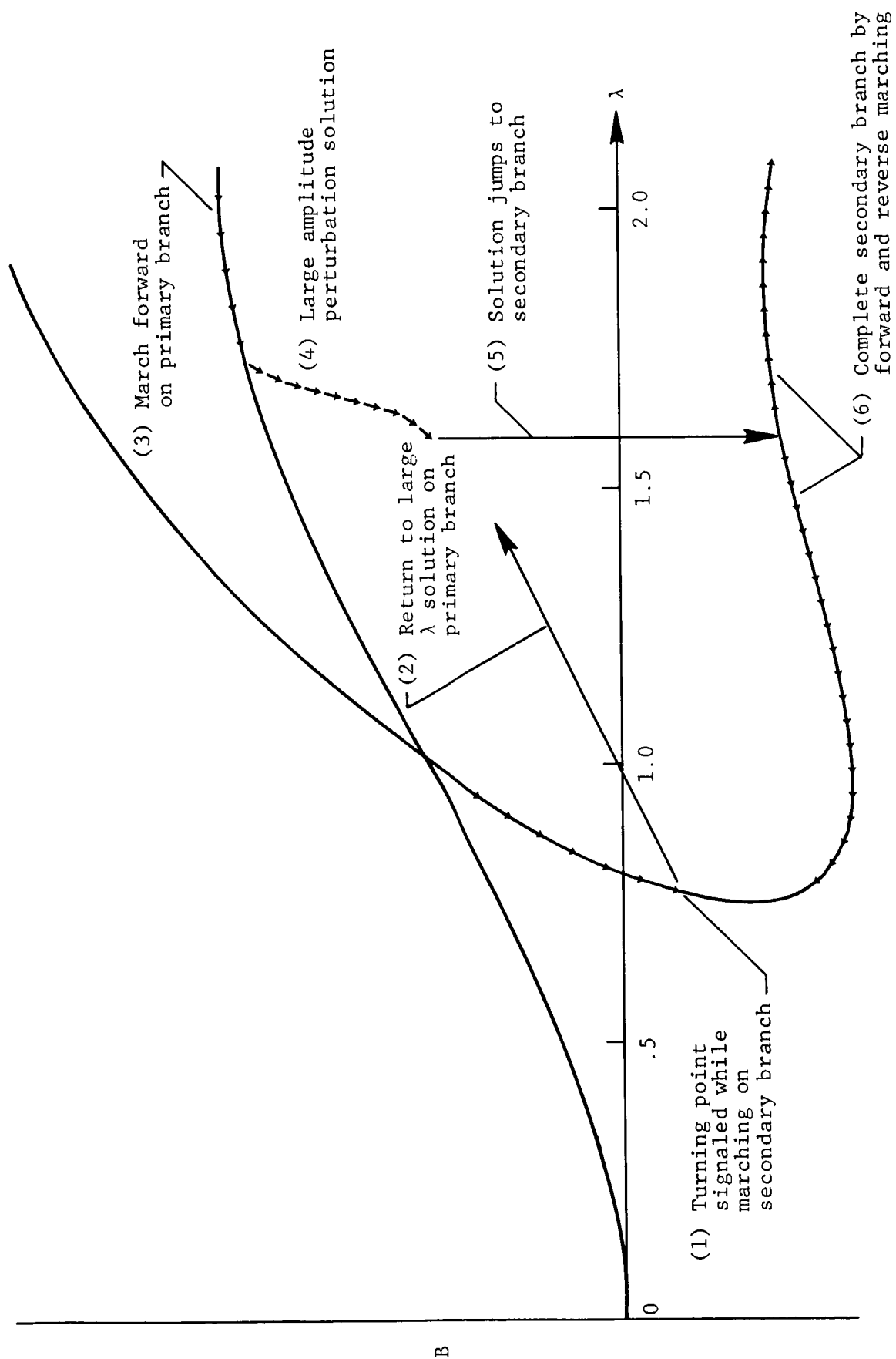


Figure 5. Perturbation technique for locating remote leg of secondary branch.

Standard Bibliographic Page

1. Report No. NASA TP-2654		2. Government Accession No.		3. Recipient's Catalog No.	
4. Title and Subtitle Some Path-Following Techniques for Solution of Nonlinear Equations and Comparison With Parametric Differentiation				5. Report Date December 1986	
				6. Performing Organization Code 505-68-91-09	
7. Author(s) Raymond L. Barger and Robert W. Walters				8. Performing Organization Report No. L-16199	
				10. Work Unit No.	
9. Performing Organization Name and Address NASA Langley Research Center Hampton, VA 23665-5225				11. Contract or Grant No.	
				13. Type of Report and Period Covered Technical Paper	
12. Sponsoring Agency Name and Address National Aeronautics and Space Administration Washington, DC 20546-0001				14. Sponsoring Agency Code	
15. Supplementary Notes Raymond L. Barger: Langley Research Center, Hampton, Virginia. Robert W. Walters: Virginia Polytechnic Institute and State University, Blacksburg, Virginia.					
16. Abstract Some path-following techniques are described and compared with other methods. Use of multipurpose techniques that can be used at more than one stage of the path-following computation results in a system that is relatively simple to understand, program, and use. Comparison of path-following methods with the method of parametric differentiation reveals definite advantages for the path-following methods. The fact that parametric differentiation has found a broader range of applications indicates that path-following methods have been underutilized.					
17. Key Words (Suggested by Authors(s)) Path following Continuation method Nonlinear differential equations Bifurcation points Turning points				18. Distribution Statement Unclassified—Unlimited Subject Category 64	
19. Security Classif.(of this report) Unclassified		20. Security Classif.(of this page) Unclassified		21. No. of Pages 14	
				22. Price A02	